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Distance spectral spread of a graph

Guanglong Yu [a,b], Hailiang Zhang [b,c], Huiqiu Lin [b], Yarong Wu [b,d], Jinlong Shu [b,*]

[a] *Department of Mathematics, Yancheng Teachers University, Yancheng, 224002, Jiangsu, China*
[b] *Department of Mathematics, East China Normal University, Shanghai, 200241, China*
[c] *Department of Mathematics, Taizhou University, Taizhou, 317000, Zhejiang, China*
[d] *SMU College of Art and Science, Shanghai Maritime University, Shanghai, 200135, China*

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ABSTRACT

Let $D(G) = (d_{i,j})_{n\times n}$ denote the distance matrix of a connected graph G with order n, where d_{ij} is equal to the distance between vertices v_i and v_j in G. The value $D_i = \sum_{j=1}^{n} d_{ij}$ $(i = 1, 2, \cdots, n)$ is called the distance degree of vertex v_i. Denote by $\varrho(G)$, $\varrho_n(G)$ the largest eigenvalue and the smallest eigenvalue of $D(G)$ respectively. The distance spectral spread of a graph G is defined to be $S_D(G) = \varrho(G) - \varrho_n(G)$. In this paper, some lower bounds on $S_D(G)$ are given in terms of distance degrees, the largest vertex degree and clique number; the spreads of $K_n, K_{\lfloor \frac{n}{2}\rfloor,\lceil \frac{n}{2}\rceil}, K_{n-\alpha}\nabla\alpha K_1, K_{1,n-1}$ are proved to be the least among all connected graphs with n vertices, all bipartite graphs with n vertices, all the graphs with both n vertices and independent number α, all trees with n vertices respectively.

1. Introduction

The distance matrix of a graph is very useful in different fields including the design of a communication network, graph embedding theory as well as molecular stability. In [1] Balaban et al. proposed the use of distance spectral radius as a molecular descriptor. And in [4], it was successfully used to infer the extent of branching and model boiling points of alkane. The problem concerning the distance spectrum of a graph is of great interest and it has been studied extensively recently (see [6,7,14,10,13,15,16], etc.).

Throughout this article, we assume that G is a simple, connected and undirected graph of order n, that is, with n vertices. Suppose the vertices of G are indexed by $v_1, v_2, \ldots, v_n$. The distance between vertices v_i and v_j of G, denoted by $\mathrm{dist}(v_i, v_j)$, is defined to be the length (i.e. the number of edges) of the shortest path from v_i to v_j. The distance matrix of G, denoted by $D(G)$, is the $n \times n$ matrix with its (i, j)-entry equal to $\mathrm{dist}(v_i, v_j)$, $i, j = 1, 2, \ldots, n$. Note that $\mathrm{dist}(v_i, v_i) = 0$, $i = 1, 2, \ldots, n$. The value $D_i = \sum_{j=1}^{n} d_{ij}$ $(i = 1, 2, \ldots, n)$ is called the distance degree of vertex v_i. The largest eigenvalue of $D(G)$ is called the distance spectral radius of G, and is denoted by ϱ. We denote by $\varrho_n(G)$ the least eigenvalue of $D(G)$. The distance spectral spread of a graph G is defined to be $S_D(G) = \varrho(G) - \varrho_n(G)$.

We now introduce some other notations. In a graph, if vertex u is adjacent to v, we denote by $u \sim v$. We denote by $N(v)$, $\deg(v)$ the neighbor set and the degree of vertex v respectively. For two vertex-disjoint graphs G_1, G_2, the *join* of the two graphs, denoted by $G_1 \nabla G_2$, is a graph obtained from the disjoint union $G_1 + G_2$ by adding edges between each vertex of G_1 and each of G_2. We denote by K_n a complete graph of order n, and denote by $K_{s,t}$ a complete bipartite graph with one part s vertices and the other part t vertices. For a graph G, we denote by $\omega(G)$, $\alpha(G)$ the clique number and the independence number respectively.

From [8,12], we know that the spread of a matrix is a very interesting topic. As a result, the spread of some matrix of a graph becomes an interesting topic in algebraic graph theory. In [3], Gregory et al. considered the (adjacency) spread of the

* Corresponding author.
E-mail addresses: yglong01@163.com (G. Yu), jlshu@math.ecnu.edu.cn (J. Shu).

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spectrum of a graph. In [9], Liu and Liu considered the signless Laplacian spread of a graph. Motivated by these, we consider the distance spread of a graph. The purpose of the present paper is to consider the bounds of $S_D(G)$ and to characterize the extremal graphs with the upper or lower bounds. Section 1 introduces the basic ideas and their supports; Section 2 gives some bounds on $S_D(G)$ in terms of the largest vertex degree, distance degree and the clique number; Section 3 proves that the spreads of $K_n, K_{\lfloor \frac{n}{2}\rfloor,\lceil \frac{n}{2}\rceil}, K_{n-\alpha} \nabla \alpha K_1, K_{1,n-1}$ are the least among all connected graphs with n vertices, all bipartite graphs with n vertices, all the graphs with both n vertices and independent number α, all trees with n vertices respectively.

2. Bounds on S_D

Definition 2.1. Let G be a simple connected graph with n vertices, $v \in V(G)$. $t_v = \frac{\sum_{v_i\sim v} D_i}{d_v}$ is called the average distance degree of v.

Lemma 2.2 (*[14]*). *The distance spectrum of the complete bipartite graph $K_{m,n}$ consists of simple eigenvalues $m+n-2 \pm \sqrt{m^2-mn+n^2}$ and an eigenvalue -2 with multiplicity $m+n-2$.*

Consider two sequences of real numbers: $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$, and $\mu_1 \geq \mu_2 \geq \cdots \geq \mu_m$ with $m < n$. The second sequence is said to interlace the first one whenever $\lambda_i \geq \mu_i \geq \lambda_{n-m+i}$ for $i = 1, 2, \ldots, m$. The interlacing is called tight if there exists an integer $k \in [1, m]$ such that $\lambda_i = \mu_i$ hold for $1 \leq i \leq k$ and $\lambda_{n-m+i} = \mu_i$ hold for $k+1 \leq i \leq m$.

Given an n by n real symmetric matrix $A_{n\times n}$ and an ordered partition $(X_1, \ldots, X_m)$ of the ordered set $\{1, 2, \ldots, n\}$, $A_{n\times n}$ can be presented as a partitioned matrix:

$$A_{n\times n} = \begin{pmatrix} A_{11} & \cdots & A_{1m} \\ \cdots & \cdots & \cdots \\ A_{m1} & \cdots & A_{mm} \end{pmatrix},$$

where A_{ij} has X_i as the set of its row numbers and X_j as the set of its column numbers. We use B hereafter to denote the quotient matrix of the partitioned real symmetric matrix $A_{n\times n}$, which is defined to be the m by m matrix whose entries are the average row sums of the blocks A_{ij}; that is, the (i, j)-entry of B is obtained by dividing the sum of all row sums of A_{ij} by $|X_i|$, where $1 \leq i, j \leq m$.

Lemma 2.3 (*[5]*). *Suppose B is the quotient matrix of a symmetric partitioned real symmetric matrix A. Then, the eigenvalues of B interlace the eigenvalues of A.*

Theorem 2.4. *Let G be a simple connected bipartite graph with n vertices, and let $S = \sum_{i=1}^{n} D_i$. Denote by Δ the largest vertex degree in G. Suppose* $\deg(v_1) = \deg(v_2) = \cdots \deg(v_k) = \Delta$. *Then*

(i) *if $\Delta \leq n-2$, then* $S_D(G) \geq \max_{1\leq i\leq k}\{\frac{\sqrt{\phi_{i,1}^2-4\phi_{i,2}(\Delta+1)(n-\Delta-1)}}{(\Delta+1)(n-\Delta-1)}\}$, *where* $\phi_{i,1} = 2(n-t_{v_i}-1)\Delta^2 + (S-2t_{v_i}-2)\Delta + S$, $\phi_{i,2} = \Delta^2(2S - t_{v_i}^2 - 2t_{v_i} - 1)$;

(ii) *if $\Delta = n-1$, then* $S_D(G) = \begin{cases} 0, & n = 1; \\ 2, & n = 2; \\ n + \sqrt{n^2-3n+3}, & n \geq 3. \end{cases}$

Proof. (i) if $\Delta \leq n-2$, for $1 \leq i \leq k$, let $N(v_i) = \{v_{i_1}, v_{i_2}, \ldots, v_{i_\Delta}\}$ and $N[v_i] = N(v_i) \bigcup \{v_i\}$. Then $V(G)$ is partitioned into two parts which are $N[v_i]$ are $V(G) \setminus N[v_i]$. Corresponding to this partition, $D(G)$ can be presented as

$$D(G) = (d_{ij})_{n\times n} = \begin{pmatrix} 0 & 1 & 1 & \cdots & 1 & \\ 1 & 0 & 2 & \cdots & 2 & \\ 1 & 2 & 0 & \cdots & 2 & * \\ \vdots & \vdots & \vdots & \ddots & \vdots & \\ 1 & 2 & 2 & \cdots & 0 & \\ & & * & & & * \end{pmatrix},$$

and the quotient matrix is as follow

$$\widetilde{D}(G) = \begin{pmatrix} \dfrac{2\Delta^2}{\Delta+1} & \dfrac{t_{v_i}\Delta + \Delta - 2\Delta^2}{\Delta+1} \\ \dfrac{t_{v_i}\Delta + \Delta - 2\Delta^2}{n-\Delta-1} & \dfrac{S - 2t_{v_i}\Delta - 2\Delta + 2\Delta^2}{n-\Delta-1} \end{pmatrix}.$$

Solving $|\lambda I - \widetilde{D}(G)| = 0$, we get the eigenvalues of $\widetilde{D}(G)$

$$\lambda_1, \lambda_2 = \frac{\phi_{i,1} \pm \sqrt{\phi_{i,1}^2 - 4\phi_{i,2}(\Delta+1)(n-\Delta-1)}}{2(\Delta+1)(n-\Delta-1)},$$

where $\phi_{i,1} = 2(n-t_{v_i}-1)\Delta^2 + (S-2t_{v_i}-2)\Delta + S$, $\phi_{i,2} = \Delta^2(2S - t_{v_i}^2 - 2t_{v_i} - 1)$. By Lemma 2.3, (i) follows.

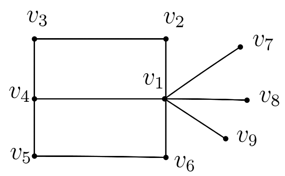

Fig. 2.1. $\mathscr{D}$.

(ii) It is trivial for $n = 1, 2$. For $n \geq 3$, it is to see that $G \cong K_{1,n-1}$. Then (ii) follows from Lemma 2.2. This completes the proof. $\square$

For an application of Theorem 2.4, we see an example as follows.

For $\mathscr{D}$ (see Fig. 2.1), $t_1 = m_D(v_1) = 16$. $\phi_{1,1} = 186$, $\phi_{1,2} = -468$. By (i) in Theorem 2.4, we get $S_D(\mathscr{D}) \geq 17.6132$. By computation with Matlab, we have $S_D(\mathscr{D}) \approx 20.9674$. This shows that Theorem 2.4 can be useful to evaluate the distance spread of a bipartite graph.

Theorem 2.5. *Let G be a simple connected graph with n vertices and clique number ω. Suppose that $G_1, G_2, \dots, G_k$ are all the cliques with order ω. Let D_j be the distance degree of vertex v_j, $S = \sum_{v_j \in V(G)} D_j$. For $1 \leq i \leq k$, let $S_{i,1} = \sum_{v_j \in V(G_i)} D_j$, $S_{i,2} = \sum_{v_j \notin V(G_i)} D_j$. Then*

(i) *if $\omega = n$, then $S_D(G) = n$;*
(ii) *if $\omega \leq n - 1$, then*

$$S_D(G) \geq \max_{1 \leq i \leq k} \left\{ \frac{\sqrt{\varphi_{i,1}^2 - 4\varphi_{i,2}\omega(n-\omega)}}{\omega(n-\omega)} \right\},$$

where $\varphi_{i,1} = \omega(S_{i,2} - S_{i,1} + n(\omega - 1))$, $\varphi_{i,2} = S\omega(\omega - 1) - S_{i,1}^2$.

Proof. (i) If $\omega = n$, then $\varrho(G) = n - 1$, $\varrho_n(G) = -1$. Hence $S_D(G) = n$.

(ii) If $\omega \leq n - 1$, for $1 \leq i \leq k$, let $V(G_i) = \{v_{i_1}, v_{i_2}, \dots, v_{i_s}\}$. Then $V(G)$ is partitioned into two parts which are $V(G_i)$ and $V(G) \setminus V(G_i)$. Corresponding to this partition, the quotient matrix of $D(G)$ is as follows

$$\widetilde{D}(G) = \begin{pmatrix} \omega - 1 & \dfrac{S_{i,1}}{\omega} - (\omega - 1) \\ \dfrac{S_{i,1} - \omega(\omega - 1)}{n - \omega} & \dfrac{S_{i,2} - S_{i,1} + \omega(\omega - 1)}{n - \omega} \end{pmatrix}.$$

Note that $S = S_{i,1} + S_{i,2}$. Solving $|\lambda I - \widetilde{D}(G)| = 0$, we get

$$\lambda_1, \lambda_2 = \frac{\varphi_{i,1} \pm \sqrt{\varphi_{i,1}^2 - 4\varphi_{i,2}\omega(n-\omega)}}{2\omega(n-\omega)},$$

where $\varphi_{i,1} = \omega(S_{i,2} - S_{i,1} + n(\omega - 1))$, $\varphi_{i,2} = S\omega(\omega - 1) - S_{i,1}^2$.

By Lemma 2.3, we get

$$S_D(G) \geq \lambda_1 - \lambda_2 \geq \frac{\sqrt{\varphi_{i,1}^2 - 4\varphi_{i,2}\omega(n-\omega)}}{\omega(n-\omega)}.$$

This completes the proof. $\square$

For an application of Theorem 2.5, we see an example as follow.

For $\mathscr{H}$ (see Fig. 2.2), $\omega = 3$, $\mathscr{H}_1 = \mathscr{H}[v_1, v_2, v_3]$ is a clique with order 3. By computation with Matlab, we get $S_D(\mathscr{H}) \approx 12.7893$. For $\mathscr{H}_1$, $S_{1,1} = 24$, $S_{1,2} = 26$, $S = 50$, $\varphi_{1,1} = 42$, $\varphi_{1,2} = -276$. By Theorem 2.5, we get $S_D(\mathscr{H}) \geq 12.0185$, which is approximated to 12.7893.

From the proof of Theorem 2.5, we get the following corollary.

Corollary 2.6. *Let G be a simple connected graph with n vertices and clique number $\omega \leq n - 1$. Suppose that $G_1, G_2, \dots, G_k$ are all the cliques with order ω. Let D_j be the distance degree of vertex v_j, $S = \sum_{v_j \in V(G)} D_j$. For $1 \leq i \leq k$, let $S_{i,1} = \sum_{v_j \in V(G_i)} D_j$, $S_{i,2} = \sum_{v_j \notin V(G_i)} D_j$, and let $\varphi_{i,1} = \omega(S_{i,2} - S_{i,1} + n(\omega - 1))$, $\varphi_{i,2} = S\omega(\omega - 1) - S_{i,1}^2$. Then*

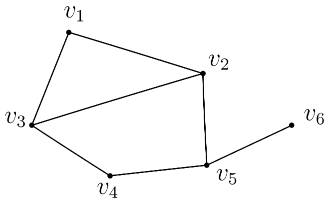

Fig. 2.2. $\mathscr{H}$.

(i) $\varrho(G) \geq \max_{1\leq i\leq k}\{\frac{\varphi_{i,1}+\sqrt{\varphi_{i,1}^2-4\varphi_{i,2}\omega(n-\omega)}}{2\omega(n-\omega)}\}$;

(ii) $\varrho_n(G) \leq \min_{1\leq i\leq k}\{\frac{\varphi_{i,1}-\sqrt{\varphi_{i,1}^2-4\varphi_{i,2}\omega(n-\omega)}}{2\omega(n-\omega)}\}$.

3. Extremal graphs with the least S_D

Lemma 3.1 ([2]). *Let H_n denotes the set of all $n\times n$ Hermitian matrices. Suppose $A \in H_n$ with eigenvalues $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$. B is a $m \times m$ principal matrix of A. Suppose B has eigenvalues $\mu_1 \geq \mu_2 \geq \cdots \geq \mu_m$. Then $\lambda_i \geq \mu_i \geq \lambda_{n-m+i}$ for $i = 1, 2, \ldots, m$.*

Lemma 3.2 ([11]). *Suppose both A, B are nonnegative irreducible and $B \leq A$ (namely $B_{i,j} \leq A_{i,j}$ for each pair of i, j). Then $\varrho(B) \leq \varrho(A)$ with equality if and only if $B = A$.*

By Lemma 3.2, we get that for an edge e of a graph G, if $G - e$ is also connected, then $\varrho(G - e) > \varrho(G)$. Conversely, if adding a new edge e to the graph G, then $\varrho(G + e) < \varrho(G)$.

Theorem 3.3. *Let G be a simple connected graph with n vertices. Then $S_D(G) \geq n$ with equality if and if only $G \cong K_n$.*

Proof. Clearly the theorem holds for the case $n \leq 2$.

Next we suppose $n \geq 3$. Then $\omega \geq 2$ and $D(K_2)$ is a principal matrix of $D(G)$. So $\varrho_n(G) \leq -1$ by Lemma 3.1. By Lemma 3.2, we get that $\varrho(G) \geq n - 1$, with equality if and only if $G \cong K_n$. Then the theorem follows immediately. This completes the proof. □

Theorem 3.4. *Let G be a simple connected bipartite graph with n vertices. Then*

$$S_D(G) \geq n + \sqrt{\left\lceil\frac{n}{2}\right\rceil^2 - \left\lfloor\frac{n}{2}\right\rfloor\left\lceil\frac{n}{2}\right\rceil + \left\lfloor\frac{n}{2}\right\rfloor^2}$$

with equality if and if only $G \cong K_{\lfloor\frac{n}{2}\rfloor,\lceil\frac{n}{2}\rceil}$.

Proof. Clearly the theorem holds for the case $n \leq 2$.

Next we suppose $n \geq 3$, $G = G[V_1, V_2]$, $|V_1| = n_1$, $|V_2| = n_2$, $n_1 + n_2 = n$. By Lemma 3.2, we get that $\varrho(G) \geq \varrho(K_{n_1,n_2})$, with equality if and only if $G \cong K_{n_1,n_2}$. And by Lemma 2.2, we get $\varrho(K_{n_1,n_2}) \geq \varrho(K_{\lfloor\frac{n}{2}\rfloor,\lceil\frac{n}{2}\rceil})$ with equality if and only if $K_{n_1,n_2} \cong K_{\lfloor\frac{n}{2}\rfloor,\lceil\frac{n}{2}\rceil}$. Note that there must be an induced subgraph $K_{1,2}$ in G. Then $D(K_{1,2})$ is a principal matrix of $D(G)$. By Lemma 2.2, we get $\varrho_3(K_{1,2}) = -2$, and by Lemma 3.1, we get $\varrho_n(G) \leq -2$. By Lemma 2.2, noting that for any bipartite graph $K_{s,t}$, we have $s + t - 2 - \sqrt{s^2 - st + t^2} > -2$ for $s + t > 0$. Hence $\varrho_n(K_{\lfloor\frac{n}{2}\rfloor,\lceil\frac{n}{2}\rceil}) = -2$. As a result, it follows that $S_D(G) \geq S_D(K_{\lfloor\frac{n}{2}\rfloor,\lceil\frac{n}{2}\rceil})$ with equality if and if only $G \cong K_{\lfloor\frac{n}{2}\rfloor,\lceil\frac{n}{2}\rceil}$. Then by Lemma 2.2, the theorem follows. This completes the proof. □

Lemma 3.5 ([14]). *For $i = 1, 2$, let G_i be an r_i-regular graph with n_i vertices and eigenvalues of the adjacency matrix A_{G_i}, $\lambda_{i,1} = r_i \geq \lambda_{i,2} \geq \lambda_{i,3} \geq \cdots \geq \lambda_{i,ni}$. The distance spectrum of $G_1 \nabla G_2$ consists of eigenvalues $-\lambda_{i,j} - 2$ for $i = 1, 2$ and $j = 2, 3, \ldots, n_i$ and two more eigenvalues of the form*

$$n_1 + n_2 - 2 - \frac{r_1 + r_2}{2} \pm \sqrt{\left(n_1 - n_2 - \frac{r_1 - r_2}{2}\right)^2 + n_1 n_2}.$$

Theorem 3.6. *Let G be a simple connected graph with n vertices and independence number α ($\alpha \leq n - 1$). Then*

(i) *for $\alpha = 1$, we have* $S_D(G) = \begin{cases} 0, & n = 1; \\ n, & n \geq 2; \end{cases}$

(ii) *for $2 \leq \alpha \leq n - 1$, we have $S_D(G) \geq n - \frac{n-\alpha-1}{2} + \frac{1}{2}\sqrt{(n - \alpha + 1)^2 + 4\alpha^2 - 4\alpha}$, with equality if and if only $G \cong K_{n-\alpha}\nabla\alpha K_1$.*

Proof. (i) If $\alpha = 1$, then G is a complete graph. It is easy to check that the theorem holds.

(ii) By Lemma 3.2, for a graph G with $2 \leq \alpha \leq n - 1$, we have $\varrho(G) \geq \varrho(K_{n-\alpha} \nabla \alpha K_1)$ with equality if and only if $G \cong K_{n-\alpha} \nabla \alpha K_1$. Noting that for positive integers n_1, n_2, r_1, if $r_1 \leq n_1 - 1$, we have

$$\left(n_1 + n_2 - \frac{r_1}{2}\right)^2 - \left(n_1 - n_2 - \frac{r_1}{2}\right)^2 - n_1 n_2 = 3n_1 n_2 - r_1 n_2 > 0,$$

which means that if $r_2 = 0$, then

$$n_1 + n_2 - 2 - \frac{r_1 + r_2}{2} - \sqrt{\left(n_1 - n_2 - \frac{r_1 - r_2}{2}\right)^2 + n_1 n_2} > -2.$$

As a result, by Lemma 3.5, if $2 \leq \alpha \leq n - 1$, we get that $\varrho_n(K_{n-\alpha} \nabla \alpha K_1) = -2$.

For a graph G with $2 \leq \alpha \leq n - 1$, we know that there must be an induced graph $K_{1,2}$. As a result, $D(K_{1,2})$ is a principal matrix of $D(G)$. Noting that by Lemma 2.2, we have $\varrho_3(K_{1,2}) = -2$. Hence, by Lemma 3.1, we get $\varrho_n(G) \leq -2$.

From above discussion, it follows immediately that for a graph G with $2 \leq \alpha \leq n - 1$, we have $S_D(G) \geq S_D(K_{n-\alpha} \nabla \alpha K_1)$ with equality if and only if $G \cong K_{n-\alpha} \nabla \alpha K_1$. Then by Lemma 3.1, the theorem follows. This completes the proof. □

Let K_n^k be the graph obtained by joining k independent vertices to one vertex of K_{n-k}.

Lemma 3.7 ([15]). *Of all the connected graphs with $n \geq 4$ vertices and k cut edges, the minimal distance spectral radius is obtained uniquely at K_n^k.*

For a tree we have the following lemma:

Lemma 3.8. *Of all the trees with n vertices, the minimal distance spectral radius is obtained uniquely at $K_{1,n-1}$.*

Proof. The lemma is trivial for $n \leq 3$. Combining with Lemma 3.7, the lemma follows. □

Theorem 3.9. *Let G be a tree with n vertices. Then*

$$S_D(G) \geq n + \sqrt{n^2 - 3n + 3}$$

with equality if and if only $G \cong K_{1,n-1}$.

Proof. It is easy to see that $G = K_1$ if $n = 1$; $G \cong K_2$ if $n = 2$; $G \cong K_{1,2}$ if $n = 3$. By Lemma 2.2, The theorem follows.

If $n \geq 4$, noting that there must be an induced subgraph $K_{1,2}$ in G, then $D(K_{1,2})$ is a principal matrix of $D(G)$. By Lemma 2.2, we get $\varrho_3(K_{1,2}) = -2$, and by Lemma 3.1, we get $\varrho_n(G) \leq -2$. By Lemma 2.2, noting that for any bipartite graph $K_{s,t}$, we have $s + t - 2 - \sqrt{s^2 - st + t^2} > -2$ for $s + t > 0$. Hence $\varrho_n(K_{1,n-1}) = -2$. Combining with Lemma 3.8, the theorem follows. □

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